METHOD AND APPARATUS FOR DETERMINING MOLECULAR CRYSTAL STRUCTURES

Abstract of the disclosure

An improved method and apparatus for determining molecular crystal structures is provided which enables molecular crystal structures to be identified using only powder diffraction data, that is considerably faster than conventional crystal modeling techniques. With the improved crystal modeling method and apparatus trial molecular crystal structures are reduced to a unique set of variables based on co-ordinates representative of the location and orientation of the molecule and where appropriate at least one co-ordinate representative of a torsion angle, bond length or bond angle. In addition, the total quantity of experimental powder diffraction data is reduced to provide a reduced representation of the diffraction data in the form of a structure factor intensity listing and covariance matrix. Trial crystal structures are postulated and each is defined using the set of variables that are used in determining a fitness of each trial structure with respect to the reduced representation of the experimental data. A trial crystal structure is output as an accurate representation of the actual crystal structure, when the fitness value for the trial structure is less than or equal to a predetermined threshold value. With the improved crystal modeling method and apparatus, identification of complex molecular crystal structures can be performed in seconds or minutes using the current generation of conventional personal computers or workstations as opposed to the hours and often days required with conventional techniques.